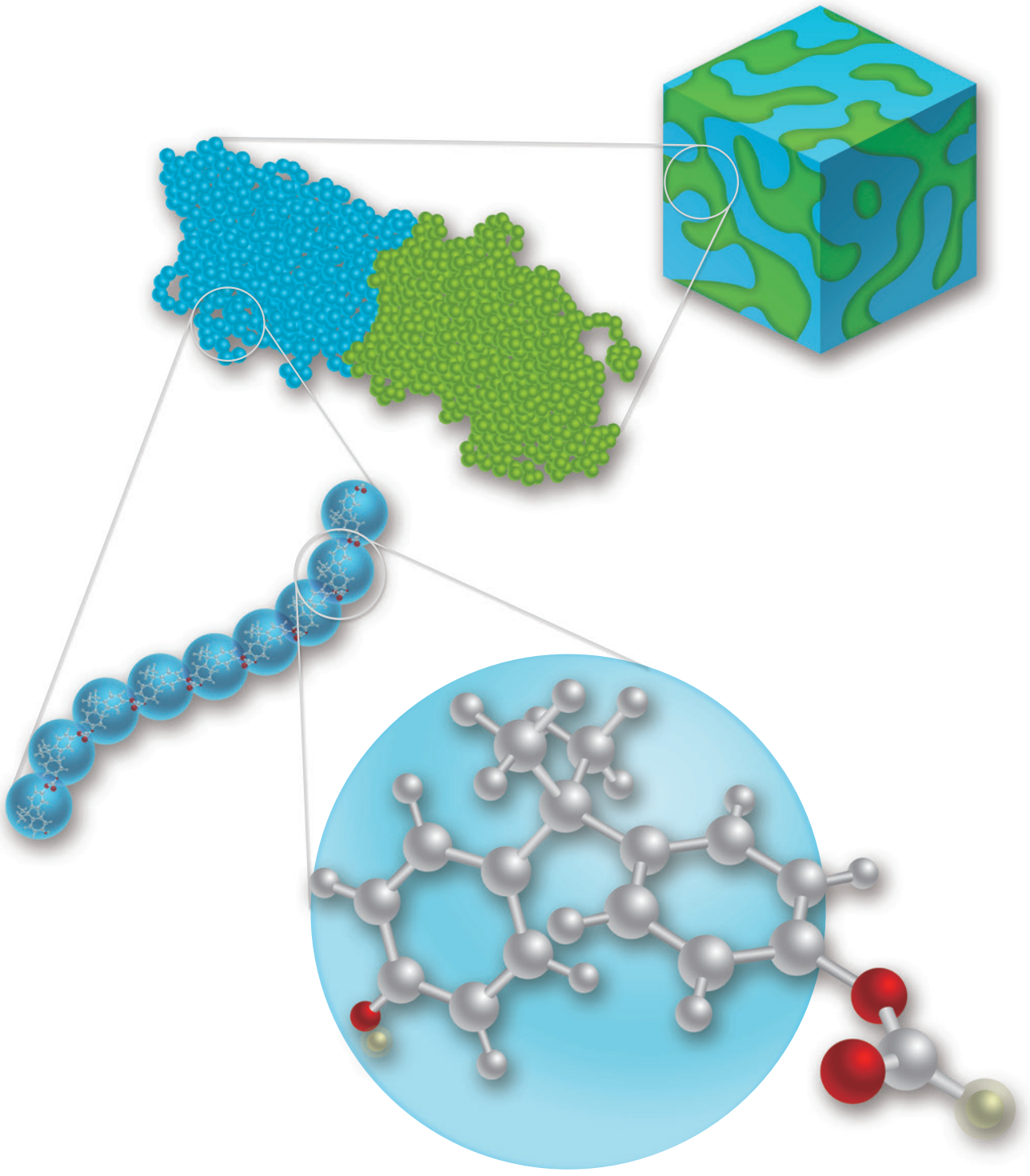
J-OCTA®

Integrated system for multiscale Modeling and Simulation



JSOL

From molecular characteristics to physical properties

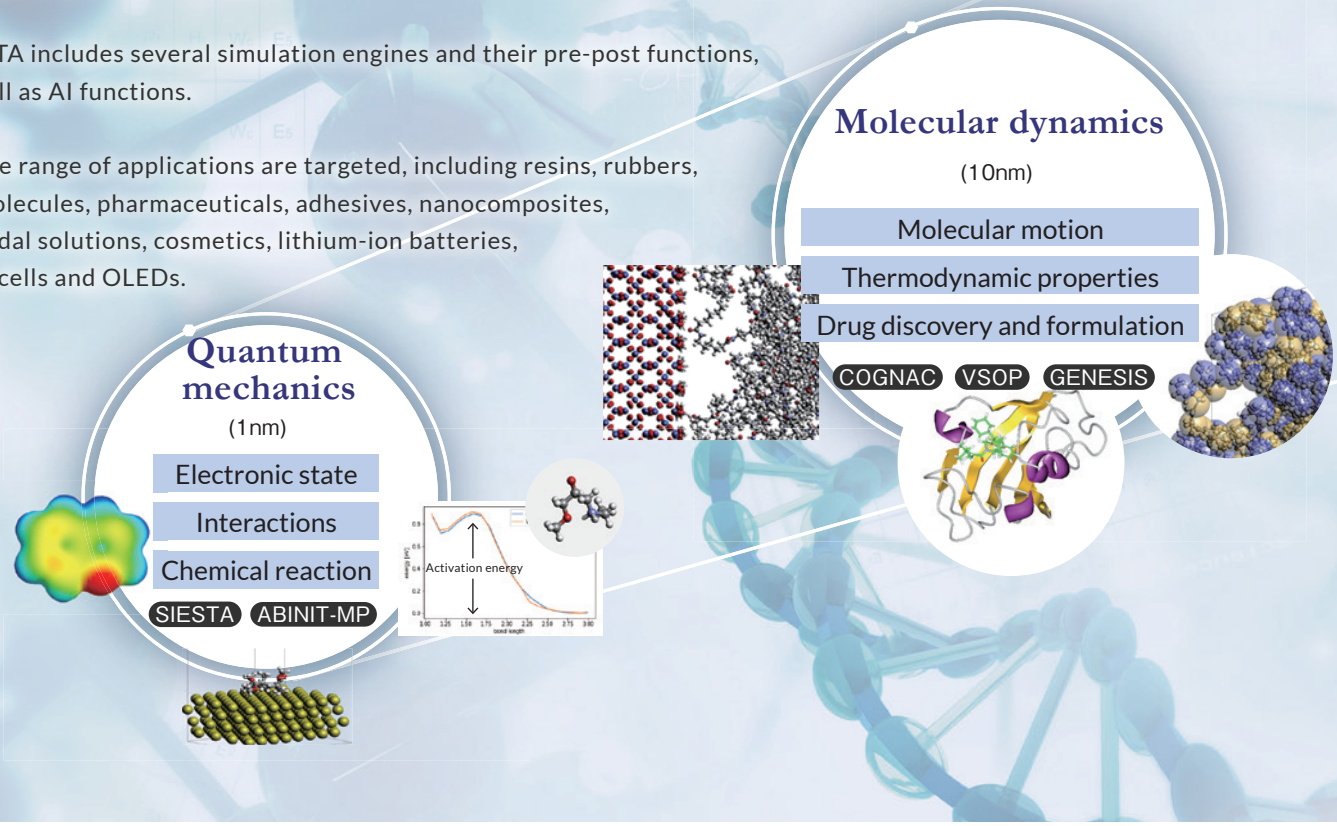
Integrated system for multiscale Modeling and Simulation

About J-OCTA®

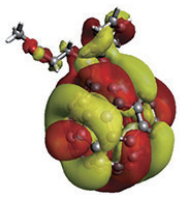
J-OCTA is a multi-scale simulation software for functional materials design and life science.
Simulators of various scales can be linked on a common platform.
Data science functions are also included to support cutting-edge research and development.

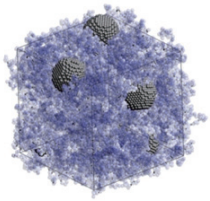
J-OCTA includes several simulation engines and their pre-post functions, as well as AI functions.

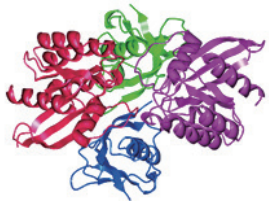
A wide range of applications are targeted, including resins, rubbers, biomolecules, pharmaceuticals, adhesives, nanocomposites, colloidal solutions, cosmetics, lithium-ion batteries, solar cells and OLEDs.

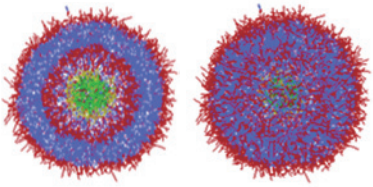


For Materials and Life sciences


Electronic state


Filler dispersion


Biomolecules


Liposome/Lipid nanoparticles

Modeling and analysis tools for materials design

- Modeling tools for molecules and crystals, coarse grained model, chemical reaction
- Many simulation engines for the evaluation of various physical properties
- Prediction of phase-separated structures, modeling of composite materials and finite element mesh generation
- Materials processing simulation such as filler dispersion, coating and evaporation

Biomolecular modeling and simulation for drug discovery and formulation

- Various modalities (small and middle-molecule, macromolecular drugs)
- Protein-ligand docking structures, free energy calculation for the evaluation of binding affinities
- Evaluation of solubility, compatibility between components
- Modeling of biological membranes, Drug delivery systems

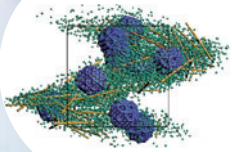
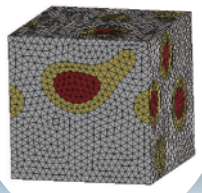
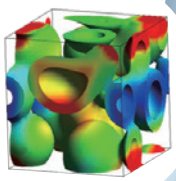
J-OCTA®

Continuum model

(1 μm)

- Composites
- Colloidal dispersion
- Thin films and Droplets

MUFFIN VSOP-PS

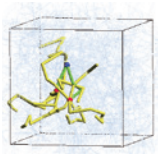
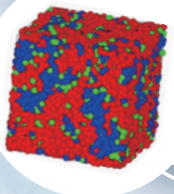
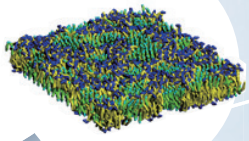




Coarse Grained model

(100nm)

- Phase separation
- Biological membranes
- Rheology

COGNAC VSOP NAPLES/PASTA SUSHI

Advantages of J-OCTA

Integrated system for multiscale Modeling and Simulation

Supports a wide range of scales from quantum to continuum. Supports selection of appropriate methods for each scale, and linkage between scales. Supports various property estimations such as mechanics, thermodynamics, optics, and electricity, as well as research targets in the fields of drug discovery and formulation.

Support for beginners

Providing the know-how necessary for molecular simulation through the case study database and scenario (workflow) functions. Even beginners can start modeling and analysis smoothly.

Support for various molecular simulation software

Providing interfaces for commonly used molecular simulation software such as Gaussian, LAMMPS, GROMACS, and etc. In addition to local execution, remote server execution or job management system are also supported.

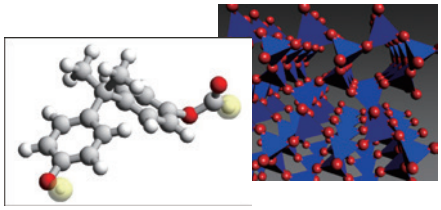
Combination of simulation and data science technologies

The strengths of each method can be used. It is possible to construct a physical property DB using the high-throughput calculation function and to predict physical properties from molecular structures using the machine learning function. Machine learning functions to accelerate simulations are also included.

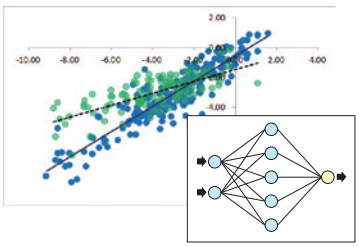
Available for Materials Design and Life Sciences

Providing easy-to-use modelers and analysis tools according to the purpose of your analysis.

Data science / Machine learning /Materials & Process Informatics



Molecules and crystal structures



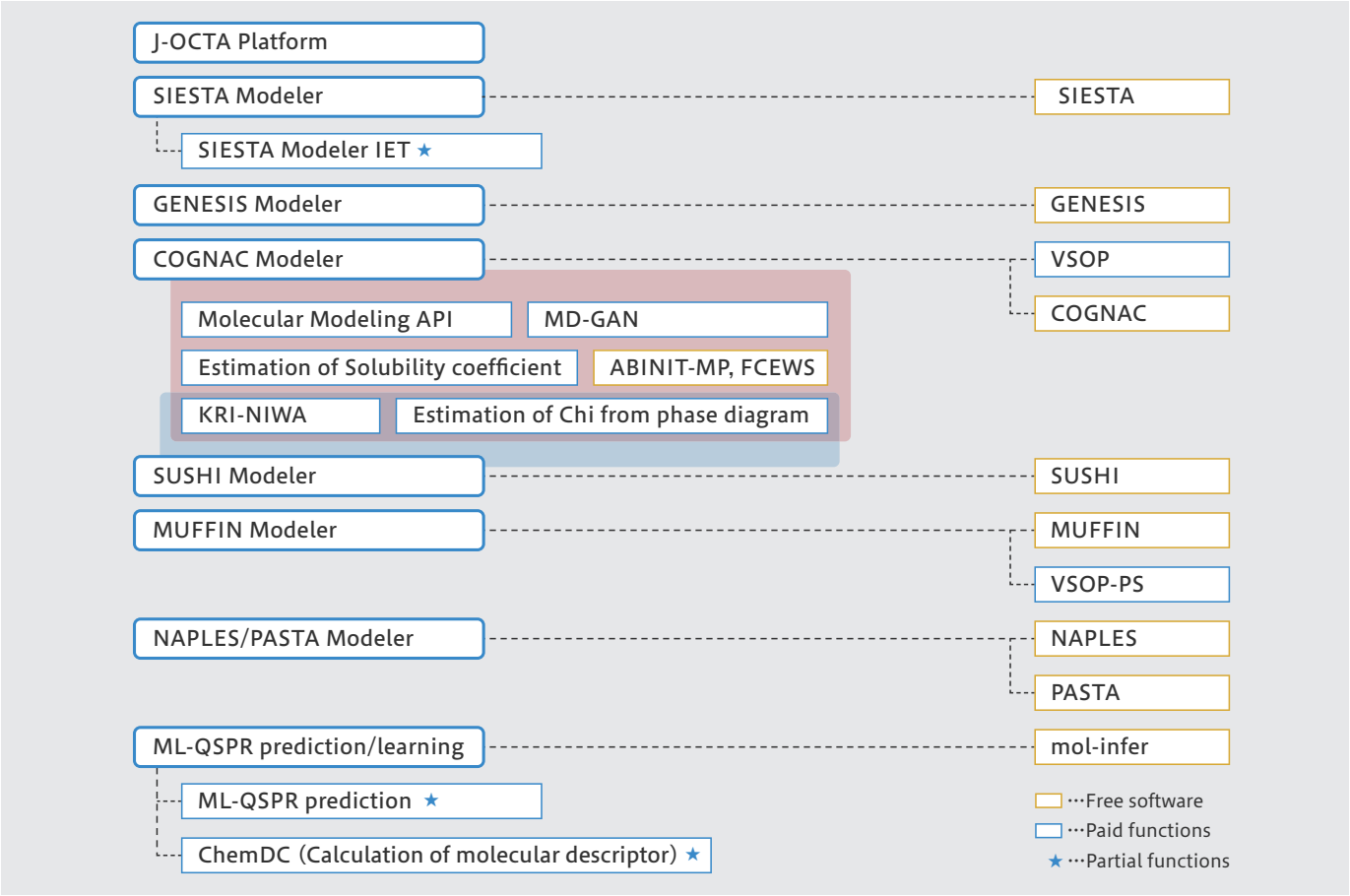
Physical properties

- Prediction of physical properties from molecular and crystal structures
- Inverse analysis to predict molecular structures from physical properties
- Supports process informatics: using process conditions for explanatory variables
- Prediction of molecular motion over long periods of time using the results of short time molecular dynamics results

- Calculation of molecular descriptors, Acquiring of physical property data from public DB
- Clustering functions such as extraction of common substructures in molecules
- Generating large amounts of physical property data by High-throughput calculations
- Support processing models and data via Python scripting

Structure of J-OCTA

To use J-OCTA's functions, "J-OCTA platform" is necessary, except for the ML-QSPR-only version.



https://octa.jp/

J-OCTA is the commercial version of the integrated simulator for soft materials, called "OCTA," that was developed through an industry-university cooperative project. OCTA is open-source software.

SIESTA is open source Density Functional Theory (DFT) software developed by a group including Universities mainly in Spain. SIESTA is a registered trade-mark of SIMUNE.

GENESIS is molecular dynamics software developed mainly by RIKEN and distributed as free software (LGPLv3).

System Requirements

	J-OCTA	Analysis Engine
OS	Windows 10 (64bit)	Windows/Linux Recommended Linux versions ・Red Hat Enterprise Linux 7 (x86-64) ・CentOS 7 (X86-64)
CPU	Multi-core CPU (recommended)	Multi-core CPU (recommended)
Memory	16 GB or more (recommended) / 8 GB (required)	16 GB or more (recommended)
Hard disk	200 GB or more free area (recommended) / 20 GB (required)	80 GB or more free area (recommended)
Display resolution	1024 X 768 or more (recommended)	
Graphics card	OpenGL-compatible graphics card (nVidia is recommended)	
Display colors	65536 colors or more (recommended)	

Support

Providing extensive seminars which ranging from basic theory to operating procedures.
Support service available by specialist staff via e-mail etc.
Assistance service will be provided during initial implementation of J-OCTA.

Contract analysis services

JSOL undertakes outsourced analysis work.
JSOL provides engineering services such as comparison/verification of analyses with experiments and advice on materials design.

Detailed information can be found on this website ▸▸▸ https://www.j-octa.com/

JSOL

NTT DATA Trusted Global Innovator NTT DATA Group

JSOL CORPORATION Engineering Technology Division

TOKYO KUDAN-KAIKAN TERRACE 1-6-5 Kudanminami, Chiyoda-ku, Tokyo 102-0074
PHONE：+81(3)6261-7168 FAX：+81(3)5210-1142

NAGOYA Marunouchi KS Bldg. 2-18-25 Marunouchi, Naka-ku, Nagoya 460-0002
PHONE：+81(52)202-8181 FAX+81(52)202-8172

OSAKA Tosabori Daibiru Bldg. 2-2-4 Tosabori, Nishi-ku, Osaka 550-0001
PHONE：+81(6)4803-5820 FAX+81(6)6225-3517

E-mail cae-info@sci.jsol.co.jp URL https://www.jsol-cae.com/en/

JOC主1E-202308